

# Equation of State of Quantum Gases Beyond the Van der Waals Approximation

K. A. Bugaev<sup>1</sup>, A. I. Ivanytskyi<sup>1</sup>, V. V. Sagun<sup>1,2</sup>, E. G. Nikonov<sup>3</sup> and G. M. Zinovjev<sup>1</sup>

<sup>1</sup>*Bogolyubov Institute for Theoretical Physics, Metrologichna str. 14<sup>B</sup>, Kiev 03680, Ukraine*

<sup>2</sup>*CENTRA, Instituto Superior Técnico, Universidade de Lisboa, Av. Rovisco Pais 1, 1049-001 Lisboa, Portugal*

<sup>3</sup>*Laboratory for Information Technologies, JINR, Joliot-Curie str. 6, 141980 Dubna, Russia*

A recently suggested equation of state with the induced surface tension is generalized to the case of quantum gases with mean-field interaction. The self-consistency conditions and the necessary one to obey the Third Law of thermodynamics are found. The quantum virial expansion of the Van der Waals models of such type is analyzed. In contrast to traditional beliefs, it is shown that an inclusion of the third and higher virial coefficients of the gas of hard spheres into the interaction pressure of the Van der Waals models either breaks down the Third Law of thermodynamics or does not allow one to go beyond the Van der Waals approximation at low temperatures. Explicitly it is demonstrated that the generalized equation of state with the induced surface tension allows one to avoid such problems and to safely go beyond the Van der Waals approximation. A few basic constraints on such models which are necessary to describe the nuclear and hadronic matter properties are discussed.

## I. INTRODUCTION

Investigation of equation of state (EoS) of strongly interacting particles at low temperatures is important for studies of the nuclear liquid-gas phase transition and for properties of neutron stars [1, 2]. To have a realistic EoS one has to simultaneously account for a short range repulsive interaction, a medium range attraction and the quantum properties of particles. Unfortunately, it is not much known about the in-medium quantum distribution functions of particles which experience a strong interaction. Therefore, a working compromise to account for all these features is to introduce the quasi-particles with quantum properties which interact via the mean-field. One of the first successful models of such type was a Walecka model [3]. However, the strong demands to consider more realistic interaction which is not restricted to some kind of effective Lagrangian led to formulating a few phenomenological approaches [4–6]. A true breakthrough among them was made in work [6] in which the hard-core repulsion was suggested for fermions.

In addition to the usual defect of the mean-field models that they break down the first and the second Van Hove axioms of statistical mechanics [7, 8] the usage of non-native variable, namely a particle number density, in the grand canonical ensemble led to formulation of the self-consistency conditions [4, 5]. In contrast to the Walecka model [3] and its followers for which the structure of Lagrangian and the extremum condition of the system pressure with respect to each mean-field automatically provide the fulfillment of the thermodynamic identities, the phenomenological mean-field EoS had to be supplemented by the self-consistency conditions [5, 9]. The latter allows one to, formally, recover the first axiom of statistical mechanics [7, 8] (for more recent discussion of the self-consistency conditions see [10–12]). An exception is given by the Van der Waals (VdW) hard-core repulsion [6], since in the grand canonical ensemble such an interaction depends on the system pressure which is the native variable for it.

Due to its simplicity the VdW repulsion is very popular in various branches of modern physics, but even in case of Boltzmann statistics it is valid at low particle densities for which an inclusion of the second virial coefficient is sufficient. For the classical gases the realistic EoS which are able to account for several virial coefficients are well-known [13, 14], while a complete quantum mechanical treatment of the third and higher virial coefficients is rather hard [15]. Hence, the quantum EoS with realistic interaction allowing one to go beyond the second virial coefficient are of great interest. It is widely believed that one possible way to reach such a goal is to include a sophisticated interaction known from the classical models [13, 14] into the mean-field models with the quantum distribution functions for quasi-particles [10, 11].

Therefore, the present work has two aims. First, we would like to analyze the popular quantum VdW models [10–12] at high and low temperatures in order to verify whether a tuning of interaction allows one to go beyond the VdW treatment. Second, we generalize to the quantum case the recently suggested EoS with the induced surface tension (IST) [16, 17] which simultaneously accounts for the second, third and fourth virial coefficients of the classical gas of hard spheres [18, 19]. Besides, we discuss a few basic constraints on quantum EoS which are necessary to model the properties of nuclear and hadronic matter.

## II. QUANTUM VIRIAL EXPANSION FOR THE VDW QUASI-PARTICLES

The typical form of EoS for quantum quasi-particles of mass  $m_p$  and degeneracy factor  $d_p$  is as follows

$$p(T, \mu, n_{id}) = p_{id}(T, \nu(\mu, n_{id})) - P_{int}(T, n_{id}), \quad (1)$$

$$p_{id}(T, \nu) = d_p \int \frac{d\mathbf{k}}{(2\pi^3)} \frac{k^2}{3} \frac{1}{E(k) e^{\left(\frac{E(k)-\nu}{T}\right)} + \zeta}, \quad (2)$$

$$\nu(\mu, n_{id}) = \mu - b p + U(T, n_{id}), \quad (3)$$

where the constant  $b \equiv 4V_0 = \frac{16\pi}{3} R_p^3$  is the excluded volume of particles with the hard-core radius  $R_p$  (here  $V_0$  is their proper volume), the relativistic energy of particle with momentum  $\vec{k}$  is  $E(k) \equiv \sqrt{\vec{k}^2 + m_p^2}$  and the density of point-like particles is defined as  $n_{id}(T, \nu) \equiv \frac{\partial p_{id}(T, \nu)}{\partial \nu}$ . The parameter  $\zeta$  switches between the Fermi ( $\zeta = 1$ ), the Bose ( $\zeta = -1$ ) and the Boltzmann ( $\zeta = 0$ ) statistics. The interaction part of pressure  $P_{int}(T, n_{id})$  and the corresponding mean-field  $U(T, n_{id})$  will be specified later.

In order to provide the validity of the thermodynamic identity  $n(T, \nu(\mu, n_{id})) \equiv \frac{\partial p(T, \nu(\mu, n_{id}))}{\partial \mu}$  for an arbitrary value of  $n_{id}(T, \nu)$ , the mean-field terms  $U$  and  $P_{int}$  should obey the self-consistency condition

$$n_{id} \frac{\partial U(T, n_{id})}{\partial n_{id}} = \frac{\partial P_{int}(T, n_{id})}{\partial n_{id}} \Rightarrow \quad (4)$$

$$P_{int}(T, n_{id}) = n_{id} U(T, n_{id}) - \int_0^{n_{id}} dn U(T, n), \quad (5)$$

After integrating by parts Eq. (4), we used in (5) an obvious condition  $U(T, 0) < \infty$ . If the condition (5) is obeyed, then the direct calculation of the  $\mu$ -derivative of the pressure (1) gives one the usual expression for particle number density in terms of the density of point-like particles

$$n = \frac{n_{id}}{1 + b n_{id}}, \quad (6)$$

$$n_{id}(T, \nu) = d_p \int \frac{d\mathbf{k}}{(2\pi^3)} \frac{1}{e^{\frac{E(k)-\nu}{T}} + \zeta}. \quad (7)$$

From these equations one finds that  $n \rightarrow b^{-1}$  for  $n_{id} \rightarrow \infty$ . The limit  $n_{id} \rightarrow \infty$  is provided by the condition  $\nu \rightarrow \infty$  for  $\zeta = \{0, 1\}$ , while for  $\zeta = -1$  it is provided by the condition  $\nu \rightarrow m_p - 0$ .

Note that in contrast to other works discussing Eqs. (4) and (5) through this paper we will use the density of point-like particles  $n_{id}$  as an argument of all functions instead of the physical density of particles  $n$  because for more sophisticated EoS their relation will be more complicated than (6). Also such a representation is convenient for a subsequent analysis because in terms of  $n_{id}(T, \nu)$  the virial expansion of  $p_{id}(T, \nu)$  looks extremely simple [15]

$$p_{id}(T, \nu) = T \sum_{l=1}^{\infty} a_l^{(0)} [n_{id}(T, \nu)]^l, \quad \text{where} \quad (8)$$

$$a_1^{(0)} = 1, \quad (9)$$

$$a_2^{(0)} = -b_2^{(0)}, \quad (10)$$

$$a_3^{(0)} = 4 [b_2^{(0)}]^2 - 2 b_3^{(0)}, \quad (11)$$

$$a_4^{(0)} = -20 [b_2^{(0)}]^3 + 18 b_2^{(0)} b_3^{(0)} - 3 b_4^{(0)}, \quad (12)$$

$$\dots\dots\dots (13)$$

Here the first few virial coefficients  $a_l^{(0)}$  of an ideal quantum gas are expressed in terms of the corresponding cluster integrals  $b_{l>1}^{(0)}$ . The latter can be expressed via the thermal density of the auxiliary Boltzmann system  $n_{id}^{(0)}(T, \nu) \equiv n_{id}(T, \nu)|_{\zeta=0}$  of Eq. (7) [15, 20]

$$b_l^{(0)} = \frac{(\mp 1)^{l+1}}{l} n_{id}^{(0)}(T/l, \nu) [n_{id}^{(0)}(T, \nu)]^{-l}, \quad (14)$$

where the upper (lower) sign corresponds to Fermi (Bose) statistics. For the non-relativistic case the expression (14) can be further simplified [15] and for an arbitrary degeneracy factor  $d_p$  it acquires the form [20]

$$b_l^{(0)} \Big|_{nonrel} \simeq \frac{(\mp 1)^{l+1}}{l^{\frac{5}{2}}} \left( \frac{1}{d_p} \left[ \frac{2\pi}{T m_p} \right]^{\frac{3}{2}} \right)^{l-1}. \quad (15)$$

For high temperatures one can write an ultra-relativistic analog of Eq. (15) for a few values of  $l = 2, 3, \dots \ll T/m_p$

$$b_l^{(0)} \Big|_{urel} \simeq \frac{(\mp 1)^{l+1}}{l^4} \left[ \frac{\pi^2}{d_p T^3} \right]^{l-1}. \quad (16)$$

Suppose that the coefficients  $a_l^{(0)}$  from Eq. (8) are known and that the virial expansion is convergent for the considered  $T$ . Then using Eq. (6) one finds  $n_{id} = n/(1 - b n)$  and, hence, one can write

$$\frac{p_{id}(T, \nu)}{T n} = \frac{1}{1 - b n} + \sum_{l=2}^{\infty} a_l^{(0)} \frac{[n]^{l-1}}{[1 - b n]^l}. \quad (17)$$

As one can see from Eqs. (15) and (16) at high temperatures all cluster integrals and virial coefficients of ideal quantum gas strongly decrease with the temperature  $T$  and, hence, at high temperatures the virial expansion of  $p_{id}(T, \nu)$  is defined by the first (classical) term on the right hand side of (17), i.e. in this case one gets

$$\frac{p_{id}(T, \nu)}{T n} \simeq 1 + 4V_0 n + (4V_0 n)^2 + (4V_0 n)^3 + \dots, \quad (18)$$

where after expanding the first term on the right hand side of (17) we used the relation between  $b$  and  $V_0$ . From this equation one sees that only the second virial coefficient,  $4V_0$ , coincides with the one for the gas of hard spheres, while the third,  $16V_0^2$ , and the fourth,  $64V_0^3$  virial coefficients are essentially larger than their counterparts  $B_3 = 10V_0^2$  and  $B_4 = 18.36V_0^3$  of the gas of hard spheres. Also Eq. (17) can naturally explain why in the work [10] the authors insisted on the interaction pressure  $P_{int}$  to be a linear function of  $T$  (see a statement after Eq. (62) in [10]): if one chooses the interaction pressure in the form

$$P_{int}(T, n(n_{id})) = T n [(b^2 - B_3)n^2 + (b^3 - B_4)n^3 + (b^4 - B_5)n^4 + \dots], \quad (19)$$

then at high temperatures the quantum corrections are negligible and, hence, for such a choice of  $P_{int}(T, n(n_{id}))$

with the corresponding value for the mean-field potential  $U(T, n(n_{id}))$  obeying the self-consistency condition (4), one can improve the total pressure of mean-field model and make its repulsive part to match the one of hard spheres.

The problem, however, arises at low temperatures, while calculating the entropy density for the model with  $P_{int}(T, n(n_{id}))$  (19). Indeed, for the choice  $U(T, n(n_{id})) = g(T)f(n(n_{id}))$  from the thermodynamic identities  $s = \frac{\partial p(T, \mu)}{\partial T}$  and  $s_{id} = \frac{\partial p_{id}(T, \nu)}{\partial T}$  one finds [10]

$$s(T, \mu) = [s_{id} + [n_{id} \frac{\partial U}{\partial T} - \frac{\partial P_{int}}{\partial T}]] [1 + b n_{id}]^{-1} = \quad (20)$$

$$\left[ s_{id} + \frac{dg(T)}{dT} \int_0^{n_{id}} d\tilde{n} f(n(\tilde{n})) \right] [1 + b n_{id}]^{-1}, \quad (21)$$

where in deriving Eq. (21) we used an explicit form of  $P_{int}$  (19) and Eq. (5). As one can see from (21) the mean-field model with linear  $T$  dependence of  $U$  or, equivalently, of  $P_{int}$ , i.e.  $g(T) = T \Rightarrow \frac{dg(T)}{dT} = 1$ , breaks down the Third Law of thermodynamics, since at  $T = 0$  one finds  $s_{id}(T = 0, \nu) = 0$  by construction, whereas  $s(T = 0, \mu) = [1 + b n_{id}]^{-1} \cdot \int_0^{n_{id}} d\tilde{n} f(n(\tilde{n})) \neq 0$ , unless  $f \equiv 0$ . Hence, the mean-field model with the linear  $T$  dependence of  $P_{int}$  may be very good at high temperatures, for which the Boltzmann statistics is valid, but it is unphysical at  $T = 0$ . Of course, one can repair this defect by choosing more complicated function  $g(T)$ , which  $g(T) \sim T$  at high  $T$ , but its derivative  $g'(T)$  vanishes at  $T = 0$  providing the fulfillment of the Third Law of thermodynamics. However, in this case the whole idea to compensate the defects of the VdW EoS by tuning the interacting part of pressure does not work at low  $T$ , since in this case  $P_{int} = g(T)F(n_{id})$  would vanish faster than the term  $T n_{id}$  on the right hand side of Eq. (17). *Thus, we explicitly showed here that at low  $T$  the mean-field models defined by Eqs. (1)-(5) either are unphysical, if  $P_{int} = TF(n_{id})$ , or they cannot go beyond the VdW approximation by adjusting their interaction pressure  $P_{int}$ .*

### III. EOS WITH INDUCED SURFACE TENSION

In order to overcome the difficulty which are faced by the mean-field models at low temperatures we suggest the following EoS

$$p = p_{id}(T, \nu_1) - P_{int1}(T, n_{id1}), \quad (22)$$

$$\Sigma = R_p [p_{id}(T, \nu_2) - P_{int2}(T, n_{id2})], \quad (23)$$

$$\nu_1 = \mu - V_0 p - S_0 \Sigma + U_1(T, n_{id1}), \quad (24)$$

$$\nu_2 = \mu - V_0 p - \alpha S_0 \Sigma + U_2(T, n_{id2}), \quad (25)$$

where  $n_{idA} \equiv \frac{\partial p_{id}(T, \nu_A)}{\partial \nu_A}$  with  $A = \{1, 2\}$ ,  $S_0 = 4\pi R_p^2$  denotes the proper surface of the hard-core volume  $V_0$ . Eq. (22) is an analog of Eq. (1), while the equation for the induced surface tension coefficient  $\Sigma$  (23) was first introduced for the Boltzmann statistics in [16]. The system

(22)-(25) is a quantum generalization of the Boltzmann EoS in the spirit of work [6]. The quantity  $\Sigma$  defined by (23) is the surface part of the hard-core repulsion [18].

Evidently, the self-consistency conditions for the IST EoS are similar to Eqs. (4) and (5)

$$n_{idA} \frac{\partial U_A(T, n_{idA})}{\partial n_{idA}} = \frac{\partial P_{intA}(T, n_{idA})}{\partial n_{idA}}, \quad A = \{1, 2\}. \quad (26)$$

The model parameter  $\alpha > 1$  is a switch between the excluded and proper volume regimes. To demonstrate this property let us consider the quantum distribution function

$$\phi_{id}(k, T, \nu_2) \equiv \frac{1}{e^{\frac{E(k) - \nu_2}{T}} + \zeta} =$$

$$\frac{e^{\frac{\nu_2 - \nu_1}{T}}}{e^{\frac{E(k) - \nu_1}{T}} + \zeta - \zeta \left[ 1 - e^{\frac{\nu_2 - \nu_1}{T}} \right]} = \phi_{id}(k, T, \nu_1) e^{\frac{\nu_2 - \nu_1}{T}} \times$$

$$\left\{ 1 + \sum_{l=2}^{\infty} \left[ \phi_{id}(k, T, \nu_1) \zeta \left( 1 - e^{\frac{\nu_2 - \nu_1}{T}} \right) \right]^l \right\}, \quad (27)$$

where in the last step of the derivation we have expanded the longest denominator above into a series of  $\phi_{id}(k, T, \nu_1) \zeta \left( 1 - e^{\frac{\nu_2 - \nu_1}{T}} \right)$  powers. Consider two limits of (27), namely  $e^{\frac{\nu_2 - \nu_1}{T}} \simeq 1$  and  $e^{\frac{\nu_2 - \nu_1}{T}} \rightarrow 0$  for  $\zeta \neq 0$ . Then the distribution function (27) can be cast as:  $\phi_{id}(k, T, \nu_2) \rightarrow$

$$\phi_{id}(k, T, \nu_1) e^{\frac{\nu_2 - \nu_1}{T}} \begin{cases} \text{with } \zeta \neq 0, & \text{if } e^{\frac{\nu_2 - \nu_1}{T}} \simeq 1, \\ \text{with } \zeta = 0, & \text{if } e^{\frac{\nu_2 - \nu_1}{T}} \rightarrow 0. \end{cases} \quad (28)$$

Further on we assume that the inequality

$$(\alpha - 1) S_0 \Sigma / n_{id2} \gg (U_2 - U_1) / n_{id2}, \quad (29)$$

holds in either of the considered limits for  $e^{\frac{\nu_2 - \nu_1}{T}}$ . Note that for the case  $e^{\frac{\nu_2 - \nu_1}{T}} \simeq 1$  the condition (29) is a natural one because at low particle densities it means that the difference of two mean-field potentials  $(U_2 - U_1)$  is weaker than the hard-core repulsion term  $(\alpha - 1) S_0 \Sigma$ ; whereas for  $e^{\frac{\nu_2 - \nu_1}{T}} \rightarrow 0$  it means that such a difference is simply restricted from above for large values of  $\Sigma$ , i.e.  $\max\{|U_1|; |U_2|\} < Const < \infty$ . Evidently, in this limit the mean-field pressures should be also finite, i.e.  $|P_{intA}| < \infty$ .

For the case  $e^{\frac{\nu_2 - \nu_1}{T}} \simeq 1$  one immediately recovers the following relation  $p_{id}(T, \nu_2) \simeq e^{\frac{(1-\alpha)S_0 \Sigma}{T}} p_{id}(T, \nu_1)$  for  $\zeta \neq 0$ , which exactly corresponds to the Boltzmann statistics version [18, 19] of the system (22)-(25) and, hence, one recovers the virial expansion of  $p_{id}(T, \nu_1)$  [18, 19] in terms of the density of particle number  $n_1 = \frac{\partial p_{id}(T, \nu_1)}{\partial \mu}|_{U_1}$  which is calculated under the condition  $U_1 = const$

$$\frac{p_{id}(T, \nu_1)}{T n_{id1}} \simeq 1 + 4V_0 n_1 + [16 - 18(\alpha - 1)] V_0^2 n_1^2 +$$

$$[64 + 121.5(\alpha - 1)^2 - 216(\alpha - 1)] V_0^3 n_1^3 + \dots \quad (30)$$

Note that due to the self-consistency condition (26) one finds  $\frac{\partial p(T, \nu_1)}{\partial \mu} = \frac{\partial p_{id}(T, \nu_1)}{\partial \mu}|_{U_1}$ , and, therefore,  $n_1$  is the physical particle number density.

As it was revealed in [18, 19] for  $\alpha = \alpha_B \equiv 1.245$  one can reproduce the fourth virial coefficient of the gas of hard spheres exactly, while the value of the third virial coefficient of such a gas is recovered with the relative error about 16% only. Therefore, for low densities, i.e. for  $V_0 n_1 \ll 1$ , the IST EoS (22)-(25) reproduces the results obtained for  $\zeta = 0$ , if the condition (29) is fulfilled.

On the other hand, from (28) one sees that in the limit  $e^{\frac{\nu_2 - \nu_1}{T}} \rightarrow 0$  the distribution function (27) with  $\zeta \neq 0$  acquires the Boltzmann form. In this limit we find  $p_{id}(T, \nu_2) \simeq p_{id}(T, \nu_1) e^{\frac{\nu_2 - \nu_1}{T}}$  and  $n_{id2}^{(0)} \simeq n_{id1}^{(0)} e^{\frac{\nu_2 - \nu_1}{T}}$ . Using these results and Eq. (29) we can rewrite (23) as

$$\Sigma \simeq R_p \left[ p_{id}(T, \nu_1) e^{\frac{(1-\alpha)S_0 \Sigma}{T}} - P_{int2}(T, n_{id2}^{(0)}) \right]. \quad (31)$$

Here we use the same notation as in previous section (see a paragraph before Eq. (14)). From Eq. (31) one can see that for  $\frac{V_0 p_{id}(T, \nu_1)}{T} \gg 1$  the surface tension coefficient  $\Sigma$  is strongly suppressed compared to  $R_p p_{id}(T, \nu_1)$ , i.e.  $\Sigma \simeq \frac{T}{S_0(\alpha-1)} \ln \left[ \frac{R_p p_{id}(T, \nu_1)}{\Sigma} \right] \ll R_p p_{id}(T, \nu_1)$ . Note that for  $\alpha > 1$  the condition  $e^{\frac{\nu_2 - \nu_1}{T}} \rightarrow 0$  can be provided by  $S_0 \Sigma / T \gg 1$  only. Thus, the second term on the right hand side of Eq. (31) cannot dominate, since it is finite. It is evident that the inequality  $\frac{V_0 p_{id}(T, \nu_1)}{T} \gg 1$  also means that  $n_{id1}^{(0)} V_0 \gg 1$ , therefore, in this limit the effective chemical potential (24) can be approximated as

$$\nu_1 \simeq \mu - V_0 p + U_1(T, n_{id1}^{(0)}), \quad (32)$$

i.e. the contribution of the induced surface tension is negligible compared to the pressure. This result means that for  $n_{id1}^{(0)} V_0 \gg 1$ , i.e. at high particle densities or for  $e^{\frac{\nu_2 - \nu_1}{T}} \rightarrow 0$ , the IST EoS corresponds to the proper volume approximation. On the other hand, Eq. (30) exhibits that at low densities, i.e. for  $e^{\frac{\nu_2 - \nu_1}{T}} \simeq 1$ , the IST EoS recovers the virial expansion up to fourth power of particle density  $n_1$ . Therefore, it is naturally to expect that for intermediate values of the parameter  $e^{\frac{\nu_2 - \nu_1}{T}} \in [0; 1]$  the IST EoS will gradually evolve from the low density approximation to the high density one, if the condition (29) is obeyed. This is a generalization of the previously obtained result [18, 19] onto the quantum statistics case.

Already from the virial expansion (30) one can see that the case  $\alpha = 1$  recovers the VdW EoS with the hard-core repulsion. If, in addition, the mean-field potentials are the same, i.e.  $U_2 = U_1$  and, consequently,  $P_{int2} = P_{int1}$ , then one finds that  $\nu_2 = \nu_1$  and  $\Sigma = R_p p(T, \nu_1)$ . In this case the term  $V_0 p + S_0 \Sigma \equiv 4V_0 p$  exactly corresponds to the VdW hard-core repulsion. If, however,  $U_2 \neq U_1$ , but both mean-field potentials are restricted from above, then the model can deviate from the VdW

EoS at low temperatures only, while at high temperatures it again corresponds to the VdW EoS. For the case  $U_2 < U_1$  this can be easily seen from Eqs. (27) and (28) for the case  $e^{\frac{\nu_2 - \nu_1}{T}} \simeq 0$ , if one sets  $\alpha = 1$ . Then using the same logic as in deriving Eq. (31), one can find that  $\Sigma \ll R_p p_{id}(T, \nu_1)$  and, hence, the effective chemical potential  $\nu_1$  acquires the form (32). In other words, at low  $T$  the surface tension effect becomes negligible and the IST EoS corresponds to the proper volume approximation, if  $e^{\frac{\nu_2 - \nu_1}{T}} \simeq 0$ .

Finally, if the inequality  $U_2 > U_1$  is valid, then at low  $T$  an expansion (27) has to be applied to the distribution function  $\phi_{id}(k, T, \nu_1)$  instead of  $\phi_{id}(k, T, \nu_2)$  and then one arrives to not very realistic case, since  $\Sigma \gg R_p p_{id}(T, \nu_1)$  and, hence, the hard-core repulsion is completely dominated by the induced surface tension term.

#### IV. GOING BEYOND VDW APPROXIMATION

Let us closely inspect the IST EoS and show explicitly its advantages over the VdW EoS. First we analyze the particle densities  $n_1(T, \nu_1) \equiv \frac{\partial p(T, \nu_1)}{\partial \mu}$  and  $n_2(T, \nu_2) \equiv R_p^{-1} \frac{\partial \Sigma(T, \nu_2)}{\partial \mu}$ . For this purpose we differentiate Eqs. (22) and (23) with respect to  $\mu$  and apply the self-consistency conditions (26)

$$n_1 = n_{id1} \left[ 1 - V_0 n_1 - S_0 \frac{\partial \Sigma}{\partial \mu} \right], \quad (33)$$

$$\frac{\partial \Sigma}{\partial \mu} = R_p n_{id2} \left[ 1 - V_0 n_1 - \alpha S_0 \frac{\partial \Sigma}{\partial \mu} \right]. \quad (34)$$

Expressing  $\frac{\partial \Sigma}{\partial \mu}$  from Eq. (34) and substituting it into (33), one finds the density of particle number

$$n_1 = \frac{n_{id1} \left( 1 - \frac{3V_0 n_{id2}}{1 + \alpha 3V_0 n_{id2}} \right)}{1 + V_0 n_{id1} \left( 1 - \frac{3V_0 n_{id2}}{1 + \alpha 3V_0 n_{id2}} \right)}, \quad (35)$$

where we used an evident relation  $R_p S_0 = 3V_0$ . From Eq. (35) one finds that for  $\alpha > 1$  the term staying in the brackets above is always positive. Therefore, irrespective of the value of  $n_{id2} \geq 0$  in the limit  $n_{id1} V_0 \gg 1$  one finds that  $\max\{n_1\} = V_0^{-1}$ . This is another way to prove that the limiting density of the IST EoS corresponds to the proper volume limit, since at high densities it is four times higher than the one of the VdW EoS.

Next we study the entropy density of the IST EoS. Similarly to finding the derivatives of Eqs. (22) and (23) with respect to  $\mu$ , one has to find their derivatives with respect to  $T$  in order to get the entropy per particle

$$\frac{s_1}{n_1} = \frac{\left[ \frac{\tilde{s}_{id1}}{n_{id1}} - \frac{3V_0 n_{id2}}{1 + \alpha 3V_0 n_{id2}} \cdot \frac{\tilde{s}_{id2}}{n_{id2}} \right]}{\left[ 1 - \frac{3V_0 n_{id2}}{1 + \alpha 3V_0 n_{id2}} \right]}, \quad (36)$$

$$\tilde{s}_{idA} \equiv s_{idA} + n_{idA} \frac{\partial U_A}{\partial T} - \frac{\partial P_{intA}}{\partial T}, \quad (37)$$

where the entropy density of point-like particles is defined as  $s_{idA} \equiv \frac{\partial p_{id}(T, \nu_A)}{\partial T}$  and  $A \in \{1; 2\}$ . If the mean-field potentials have the form  $U_A = \sum_{\lambda} g_A^{\lambda}(T) f_A^{\lambda}(n_{idA})$  and for  $T = 0$  their derivatives obey the condition  $\frac{dg_A^{\lambda}(T)}{dT} = 0$ , then it is easy to see that the entropy per particle  $\frac{s_1}{n_1}$  also vanishes at  $T = 0$ , i.e. the Third Law of thermodynamics is obeyed under these conditions.

Apparently, to provide a positive value of entropy per particle  $\frac{s_1}{n_1}$  one has to properly choose the interaction terms in Eqs. (22) and (23). It is clear that the corresponding necessary conditions should not be very restrictive because at low densities, i.e. for  $3V_0 n_{id2} \ll 1$ , the coefficient staying in front of the term  $\frac{\tilde{s}_{id2}}{n_{id2}}$  is very small, while at high densities it is  $\alpha^{-1} < 1$  for  $\alpha > 1$ . Although, a discussion of such conditions is far beyond the scope of this work, below we consider two important cases.

For the case  $U_2(T, \rho) \equiv U_1(T, \rho)$  the condition (29) is valid for any choice of parameters. Then one can show a validity of the inequality  $\frac{s_{id1}}{n_{id1}} \geq \frac{s_{id2}}{n_{id2}}$ , since for  $\alpha > 1$  one finds  $\nu_1 > \nu_2$ . For this one has to account that  $p_{id}(T, \nu_A)$  and all its derivatives are monotonously increasing functions of  $T$  and  $\nu_A$ . Then, using the relations (27) and (28) between the quantum distribution functions, one can show the validity of the inequality  $\frac{s_{id1}}{n_{id1}} \geq \frac{s_{id2}}{n_{id2}}$  for two limits  $e^{\frac{\nu_2 - \nu_1}{T}} \simeq 1$  and  $e^{\frac{\nu_2 - \nu_1}{T}} \rightarrow 0$ . Similarly, one can introduce an effective parameter of statistics  $\zeta_{eff} \equiv \zeta - \zeta \left[1 - e^{\frac{\nu_2 - \nu_1}{T}}\right]$  and study the quantities for the distribution function  $\phi_{id}(k, T, \nu_2)$  with an effective parameter of statistics  $\zeta_{eff}$ . However, one can easily understand that the inequality  $\frac{s_{id1}}{n_{id1}} \geq \frac{s_{id2}}{n_{id2}}$  cannot be broken down for the intermediate values of parameter  $e^{\frac{\nu_2 - \nu_1}{T}}$ , i.e. for  $0 < e^{\frac{\nu_2 - \nu_1}{T}} < 1$ , since the pressure of point-like particles and its partial derivatives are monotonic functions of parameters and that a non-monotonic behavior of the entropy per particle can be caused by the phase transition, which does not exist for an ideal gas. Note that here we do not consider a possible effect of the Bose-Einstein condensation. Using the above inequality between the entropies per particle and requiring that  $U_1 \geq 0$  and the inequalities  $\frac{dg_A^{\lambda}(T)}{dT} > 0$  for  $T > 0$  and  $\frac{dg_A^{\lambda}(T=0)}{dT} = 0$  one can show that  $\frac{s_1}{n_1} \geq \frac{\tilde{s}_{id2}}{n_{id2}} \geq 0$  using an identity (5).

Another important case corresponds to the choice  $U_1 > 0$  and  $U_2 < 0$ , i.e. the mean-field  $U_1$  describes an attraction, while  $U_2$  represents a repulsion. Clearly, the condition (29) in this case is also fulfilled for any choice of parameters. Using the self-consistency relations (26), or its more convenient form (5), one can find that the term describing the entropy of mean-field in  $\tilde{s}_{id2}$  is negative, i.e.  $n_{id2} \frac{\partial U_2}{\partial T} - \frac{\partial P_{int2}}{\partial T} = \sum_{\lambda} \frac{dg_2^{\lambda}(T)}{dT} \int_0^{n_{id2}} dn f_2^{\lambda}(n) < 0$ , if

$g_2^{\lambda}(T) > 0$  and  $\frac{dg_2^{\lambda}(T)}{dT} > 0$  for  $T \geq 0$ . Such a choice of interaction allows one to decrease the effective entropy density  $\tilde{s}_{id2}$  or even to make it negative by tuning the mean-field  $U_2$  related to the IST coefficient. As a result

this would increase the entropy density  $s_1$ . Note that for the VdW EoS this is impossible.

## V. APPLICATION TO NUCLEAR AND HADRONIC MATTER

As a pedagogical example we consider the IST EoS for the nuclear matter and compare it with the VdW EoS (1) having the following interaction

$$P_{int}^{VdW}(T, n_{id}) = a \left[ \frac{n_{id}}{1 + b n_{id}} \right]^2 + T n_{id} - \frac{g(T) n_{id}}{1 + b n_{id}} - \frac{g(T) b n_{id}^2}{[1 + b n_{id}]^2} - \frac{g(T) B_3 n_{id}^3}{[1 + b n_{id}]^3} - \frac{g(T) B_4 n_{id}^4}{[1 + b n_{id}]^4}, \quad (38)$$

where the virial coefficients  $b$ ,  $B_3$  and  $B_4$  are introduced above and the function  $g(T) \equiv \frac{T^2}{T + T_{SW}}$  with  $T_{SW} = 1$  MeV provides the fulfillment of the Third Law of thermodynamics. Note that the term  $T n_{id}$  cancels exactly the first term of the quantum virial expansion for  $p_{id}(T, \nu)$  (see Eq. (17)), while the term  $a \left[ \frac{n_{id}}{1 + b n_{id}} \right]^2$  in Eq. (38) accounts for an attraction and the other terms proportional to  $g(T)$  are the lowest four powers of the virial expansion for the gas of classical hard spheres for  $T \gg T_{SW}$ .

For the IST EoS we choose  $\alpha = 1.245$  [19],  $P_{int1}^{IST} = a \left[ \frac{n_{id1}}{1 + b n_{id1}} \right]^2$  and  $P_{int2}^{IST} = 0$  with the constants  $a \simeq 329$  MeV fm<sup>3</sup> and  $b = 4V_0 \simeq 3.44$  fm<sup>3</sup> which were found in [11] for VdW EoS of nuclear matter. In Fig. 1 we compare three isotherms  $T = 19, 10$  and  $0$  MeV of these two EoS. For  $T = 0$  and  $T = 19$  MeV isotherms the both models agree up to the packing fraction  $\eta = b n \simeq 0.13$  (for the density  $n \leq 0.035$  fm<sup>-3</sup>), i.e. within the usual range of the VdW EoS applicability [17–19]. For  $T = 10$  MeV their isotherms agree up to essentially higher packing fraction  $\eta \simeq 0.35$  due to the presence of four terms of virial expansion of the gas of hard spheres in Eq. (38) for VdW EoS and due to the minor role of the second and higher order quantum virial coefficients  $a_{k \geq 2}^{(0)}$  defined by Eqs. (10)–(15).

Recently an interesting generalization of the quantum VdW EoS (GVdW hereafter) was suggested in [21]. This EoS allows one to go beyond the VdW approximation, but formally it is similar to the VdW models discussed above. In terms of the ideal gas pressure (2) the GVdW pressure can be written as [21] ( $\eta = V_0 n$  is the packing fraction):

$$p_G(T, \mu) = w(\eta) p_{id}(T, \nu_G) - P_{intG}(n), \quad (39)$$

$$\nu_G(\mu, n) = \mu + V_0 f'(\eta) p_{id}(T, \nu_G) + U_G(n), \quad (40)$$

where  $n$  is the particle density, and the multiplier  $w(\eta) \equiv (f(\eta) - \eta f'(\eta))$  is given in terms of the function  $f(\eta)$  which for the VdW case is  $f^{VdW}(\eta) = 1 - 4\eta$  and for the Carnahan-Starling (CS) EoS is  $f^{CS}(\eta) = \exp \left[ -\frac{(4-3\eta)\eta}{(1-\eta)^2} \right]$ . The interaction terms of the GVdW EoS

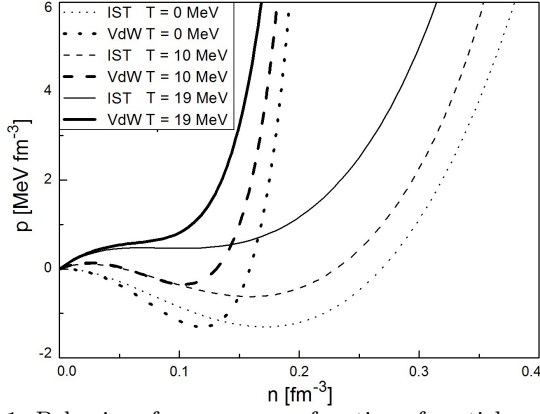


FIG. 1: Behavior of pressure as a function of particle number density for isotherms of nuclear matter (see text for details).

are given in terms of a function  $u(n)$ :  $U_G = u(n) + nu'(n)$  and  $P_{intG} = -n^2 u'(n)$ . Such a choice automatically provides the self-consistency condition fulfillment. Since the potentials  $U_G$  and  $P_{intG}$  are temperature independent, the Third Law of thermodynamics is obeyed by construction.

The presence of the function  $w(\eta)$  in front of the ideal gas pressure in (39) allows one to reproduce the CS EoS at high temperatures, while it creates the problems with formulating the GVdW model for several hard-core radii. Indeed, using the quantum virial expansion (8) and the particle number density expression  $n = f(\eta) n_{id}(T, \nu_G)$  [21], for  $P_{IG} \equiv w(\eta) p_{id}(T, \nu_G)$  one obtains

$$P_{IG} = w(\eta) T \left[ \frac{n}{f(\eta)} + \sum_{l=2}^{\infty} a_l^{(0)} [n_{id}(T, \nu_G)]^l \right], \quad (41)$$

$$\frac{w(\eta)}{f(\eta)} = \begin{cases} \frac{1}{1-4\eta} \equiv \frac{1}{f^{VdW}(\eta)}, & \text{for VdW EoS,} \\ \frac{1+\eta+\eta^2-\eta^3}{(1-\eta)^3}, & \text{for CS EoS.} \end{cases} \quad (42)$$

These equations show that due to the multiplier  $w(\eta)$  the first term of the quantum virial expansion in Eqs. (41), (8) and (17), i.e. the classical term, exactly reproduces the pressure of corresponding classical EoS. Hence, all other terms in Eqs. (8), (17) and (41) are the quantum ones. From Fig. 2 one can see that the quantum compressibility factors  $\Delta Z_Q^{CS}(\eta) = \frac{P_{IG} - w(\eta) T n_{id}(T, \nu_G)}{T n}$  for the CS EoS of the GVdW model and the one for the IST EoS  $\Delta Z_Q^{IST}(\eta) = \frac{p_{id1} - T n_{id1}(T, \nu_1)}{T n_1}$  differ already at  $\eta \simeq 0.05$ . Thus, for  $\eta \geq 0.2$  both the classical and the quantum parts of the IST pressure with  $\alpha = 1.245$  [19] are essentially softer than the corresponding terms of the CS EoS of Ref. [21].

Let's now to discuss a few basic constraints on the considered mean-field models which are necessary to describe the strongly interacting matter properties. According to Eqs. (17) and (41) the repulsive part of fermionic pressure consists of three contributions: the classical pressure  $T n_{id}$  and the quantum part of pressure; and the repulsive part of the mean-field  $P_{int}$ . At temperatures below 1 MeV the classical part is negligible. Since the true virial coefficients for the interacting quantum gases are

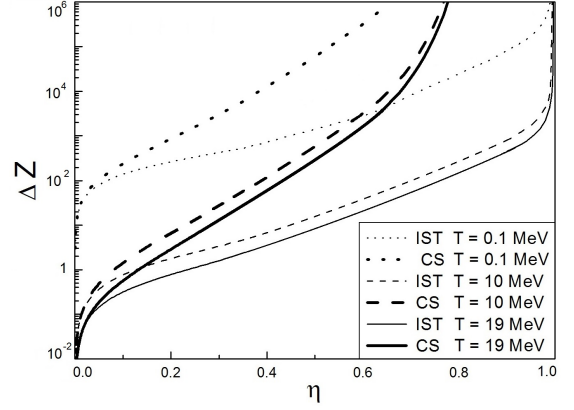


FIG. 2: Packing fraction dependence of the quantum compressibility factors  $\Delta Z_Q$  of the GVdW EoS and IST EoS (see text).

not known, it is evident that the quantum pressure of all considered models are effective by construction. To fix their parameters one has to reproduce the usual properties of normal nuclear matter, i.e. to get a zero value for the total pressure at normal nuclear density  $n_0 \simeq 0.16 \text{ fm}^{-3}$  and the binding energy  $W = -16 \text{ MeV}$  at this density [1]. In addition there is the so called flow constraint at nuclear densities  $n = (2-5)n_0$  [22], which sets strong restrictions on the model pressure dependence on nuclear particle density and requires rather soft EoS at  $n = (2-5)n_0$ . Fig. 2 shows that the existing version of the CS EoS of Ref. [21] is very stiff and, hence, it will have troubles to obey the flow constraint [22], while this is not a problem for the IST EoS [26].

From the virial expansions of all models discussed here one sees that the EoS calibration on the properties of nuclear matter at low T and at high densities involves mainly the quantum and the mean-field pressures, but, unfortunately, it also fixes the parameters of the classical pressure at higher temperatures. It is, however, clear that the one component mean-field models of nuclear matter cannot be applied at temperatures above 50 MeV, since one has to include the mesons, other baryons and their resonances [20, 23]. Moreover, in this case the mean-fields and the parameters of interaction should be recalibrated because the very fact of resonance existence already corresponds to partial accounting of the interaction [23]. For many years it is well known that for temperatures below 170 MeV and densities below  $n_0$  the mixture of stable hadrons and their resonances whose interaction is taken into account by the quantum second virial coefficients behaves as the mixture of nearly ideal gases of stable particles which, in this case, include both the hadrons and the resonances, but taken with their averaged masses [23]. The main reason for such a behavior is rooted in a nearly complete cancellation between the attraction and repulsion contributions. The resulting deviation from the ideal gas (a weak repulsion) is usually described in the hadron resonance gas model (HRGM) [17–19, 24, 25] by the classical second virial coefficients.

We have to stress that the fact of weak repulsion between the hadrons is naturally encoded in the smaller values of their hard-core radii ( $R_p < 0.4$  fm) obtained within the HRGM compared to the larger hard-core radius of nucleons in nuclear matter ( $R_n \geq 0.52$  fm [21]). Hence, in contrast to Ref. [21], we do not see any reason to believe that the mean-field model describing the nuclear matter properties may set any strict conditions on the hadronic hard-core radii of the HRGM.

Moreover, we would like to point out that a great success achieved recently by the HRGM [17–19, 24, 25] sets a strong constraint on any model of hadronic phase which pretends to be called realistic. Any such a model should reproduce the pressure, entropy and all charge densities obtained by the HRGM at the curve of chemical freeze-out  $\mu = \mu_{CFO}(T)$ . In particular, for the mean-field models discussed here it means that they should be extended in order to include all other hadrons and that at the curve  $\mu = \mu_{CFO}(T)$  the total interaction pressure must vanish, i.e.  $P_{int} = 0$ , since it does not exist in the HRGM. In other words, if at the chemical freeze-out curve such a model has nonvanishing attraction, then it must have an additional repulsion to provide  $P_{int} = 0$ . Only this condition will make a direct connection between the realistic EoS and the hadron multiplicities measured in heavy ion collisions. It is clear, that without  $T$ -dependent mean-field interaction  $P_{int}$  such a condition cannot be fulfilled. Also we have to add that the IST EoS for quantum gases is well suited for this task due to additive pressure  $p_{id}(T, \nu_{1,2})$ , whereas the generalization of the CS EoS of Ref. [21] to a multicomponent case looks rather problematic, since the CS EoS [13] is the one component EoS by construction.

## VI. CONCLUSIONS

The self-consistent generalization of the IST EoS for quantum gases is worked out. It is shown that with this

EoS one can go beyond the VdW approximation at any temperature. The restriction on the temperature dependence of the mean-field potentials are discussed. It is found that at low temperatures these potentials either should be  $T$ -independent or should vanish faster than the first power of temperature providing the fulfillment of the Third Law of thermodynamics. The same is true for the quantum VdW EoS. Hence, the idea to improve the quantum VdW EoS by tuning the interacting part of pressure [10, 11] is disproved for low temperature  $T$ : if this part of pressure is linear in  $T$ , then the VdW EoS breaks down the Third Law of thermodynamics; if it vanishes faster than the linear  $T$ -dependence, then the interaction part of pressure is useless, since it vanishes faster than the first term of the quantum virial expansion. An alternative EoS [21] allowing one to abandon the VdW approximation for nuclear matter is analyzed. The general constraints on realistic EoS for nuclear and hadronic matter are discussed and some practical conclusions are given. Based on the revealed properties of the IST EoS for quantum gases we hope that it will allow one to go far beyond the traditional VdW approximation and due to its advantages it will become a useful tool for heavy ion physics and for nuclear astrophysics.

**Acknowledgments.** The authors appreciate the valuable comments of D. B. Blaschke and R. Emaus. K.A.B., A.I.I., V.V.S. and G.M.Z. acknowledge a partial support of the Program ‘Nuclear Matter Under Extreme Conditions’ launched by the Section of Nuclear Physics of National Academy of Sciences of Ukraine. K.A.B. and A.I.I. acknowledge a warm hospitality of the University of Oslo, Norway, where this work was completed.

- 
- [1] N. K. Glendenning, “Compact Stars”, Springer-Verlag, New York 2000.
  - [2] S. Typel et al., Phys. Rev. C **81**, (2010) 015803.
  - [3] J. D. Walecka, Annals Phys. **83**, (1974) 491.
  - [4] J. Zimanyi et al., Nucl. Phys. A **484**, (1988) 647.
  - [5] K. A. Bugaev and M. I. Gorenstein, Z. Phys. C **43**, (1989) 261.
  - [6] D. H. Rischke, M. I. Gorenstein, H. Stöcker and W. Greiner, Z. Phys. C **51**, (1991) 485.
  - [7] L. Van Hove, Physica **15**, (1949) 951.
  - [8] L. Van Hove, Physica **16**, (1950) 137.
  - [9] M. I. Gorenstein et al. J. Phys. G191993L69.
  - [10] D. Anchishkin and V. Vovchenko, arXiv:1411.1444 [nucl-th] and references therein.
  - [11] V. Vovchenko, D. V. Anchishkin and M. I. Gorenstein, Phys. Rev. C **91**, (2015) 064314.
  - [12] K. Redlich and K. Zalewski, Acta Phys. Polon. B **47**, (2016) 1943.
  - [13] N. F. Carnahan and K. E. Starling, J. Chem. Phys. **51**, (1969) 635.
  - [14] J. P. Hansen and I. R. McDonald, “Theory of simple liquids”, Academic, London (2006).
  - [15] K. Huang, “Statistical mechanics”, Wiley & Sons(1963).
  - [16] V. V. Sagun, K. A. Bugaev, A. I. Ivanytskyi and I. N. Mishustin, Nucl. Phys. A **924**, (2014) 24.
  - [17] K. A. Bugaev et al., arXiv:1611.07349 [nucl-th].
  - [18] V. V. Sagun et al., arXiv:1611.07071 [nucl-th].
  - [19] V. V. Sagun et al., arXiv:1703.00049 [hep-ph].
  - [20] A. Kostyuk, M. I. Gorenstein, H. Stöcker and W. Greiner, Phys. Rev. C **63**, (2001) 044901.
  - [21] V. Vovchenko, arXiv:1701.06524 [nucl-th].
  - [22] P. Danielewicz, R. Lacey and W. G. Lynch, Science **298**, (2002) 1592.
  - [23] R. Venugopalan and M. Prakash, Nucl. Phys. A **546**,

- (1992) 718.
- [24] A. Andronic, P. Braun-Munzinger and J. Stachel, Nucl. Phys. A **772**, (2006) 167 and references therein.
- [25] K. A. Bugaev et al., Europhys. Lett. **104**, (2013) 22002.
- [26] A. I. Ivanytskyi et al., (in preparation).